Supplementary information

Crystal Growth, Single Crystal Structure and Biological Activity of Thiazolo-Pyridine Dicarboxylic Acid Derivatives

Hamdi Ben Yahia,[a] Souhir Sabri,[a] Rachid Essehli,[b] Peter Kasak,[c] Joanna Drogosz,[d] Anna Janecka,[d] and Brahim El Bali[e]*

[a]*Qatar Environment and Energy Research Institute (QEERI 2.0), Hamad Bin Khalifa University, Qatar Foundation, P.O. Box 34110 Doha, Qatar.*

[b]*Energy and Transportation Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA.*

[c]*Centre for Advanced Materials (CAM), Qatar University, 2713, Doha, Qatar.*

[d]*Department of Biomolecular Chemistry, Medical University of Lodz, Mazowiecka 6/8, 92-215 Lodz, Poland.*

[e]*Independent scientist, ORCID: 0000-0001-6926-6286; Email: b_elbali@yahoo.com*

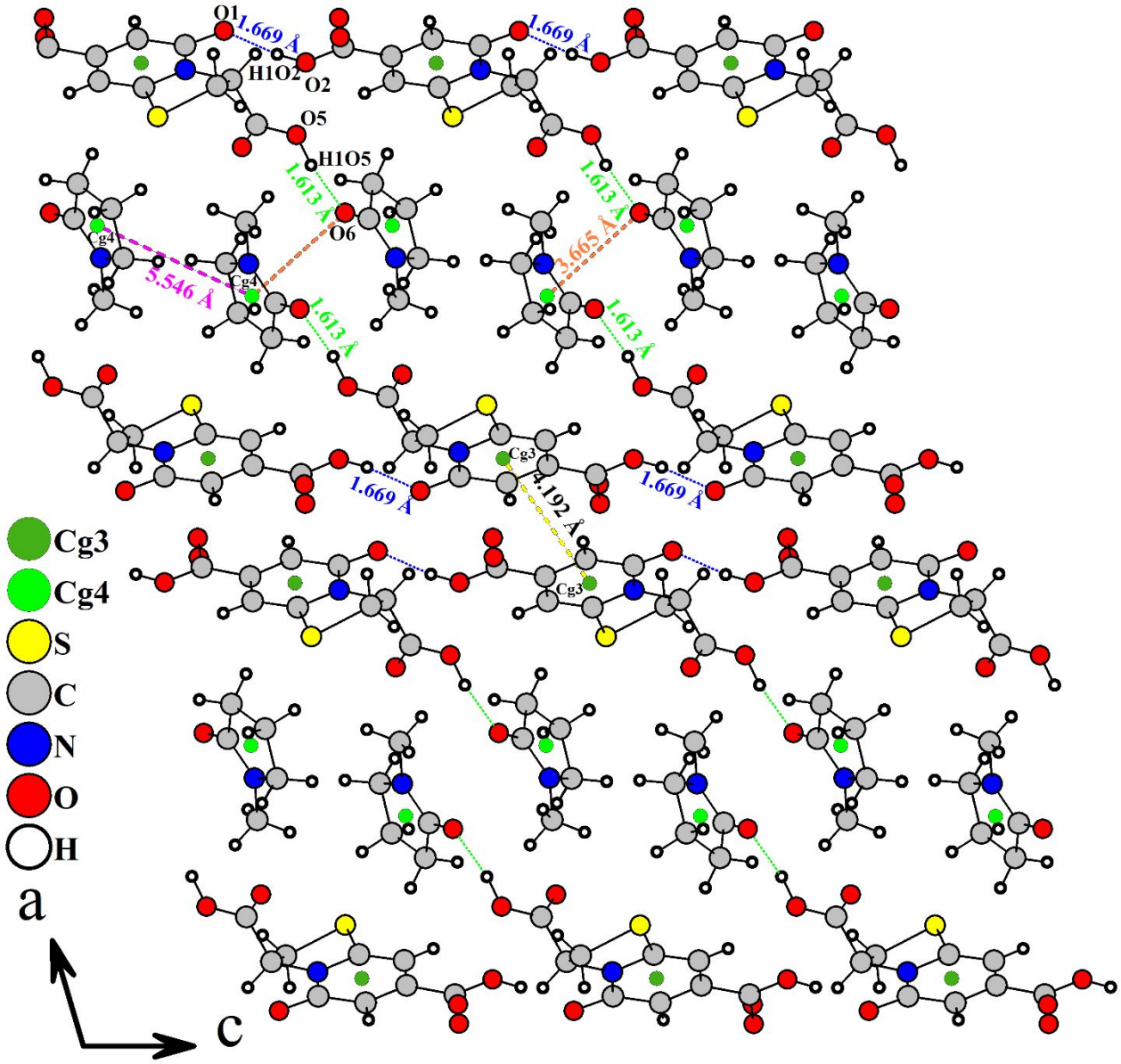

Figure S1. View of the structure of (**2**) down the *b* axis showing intermolecular interactions. The blue and green dashed lines connect TPDCA to TPDCA and NMP molecules, respectively. The brown lines correspond to C=O···π interactions within the NMP layer. The yellow and pink dashed lines emphasize the long Cg3-Cg3 and Cg4-Cg4 distances.

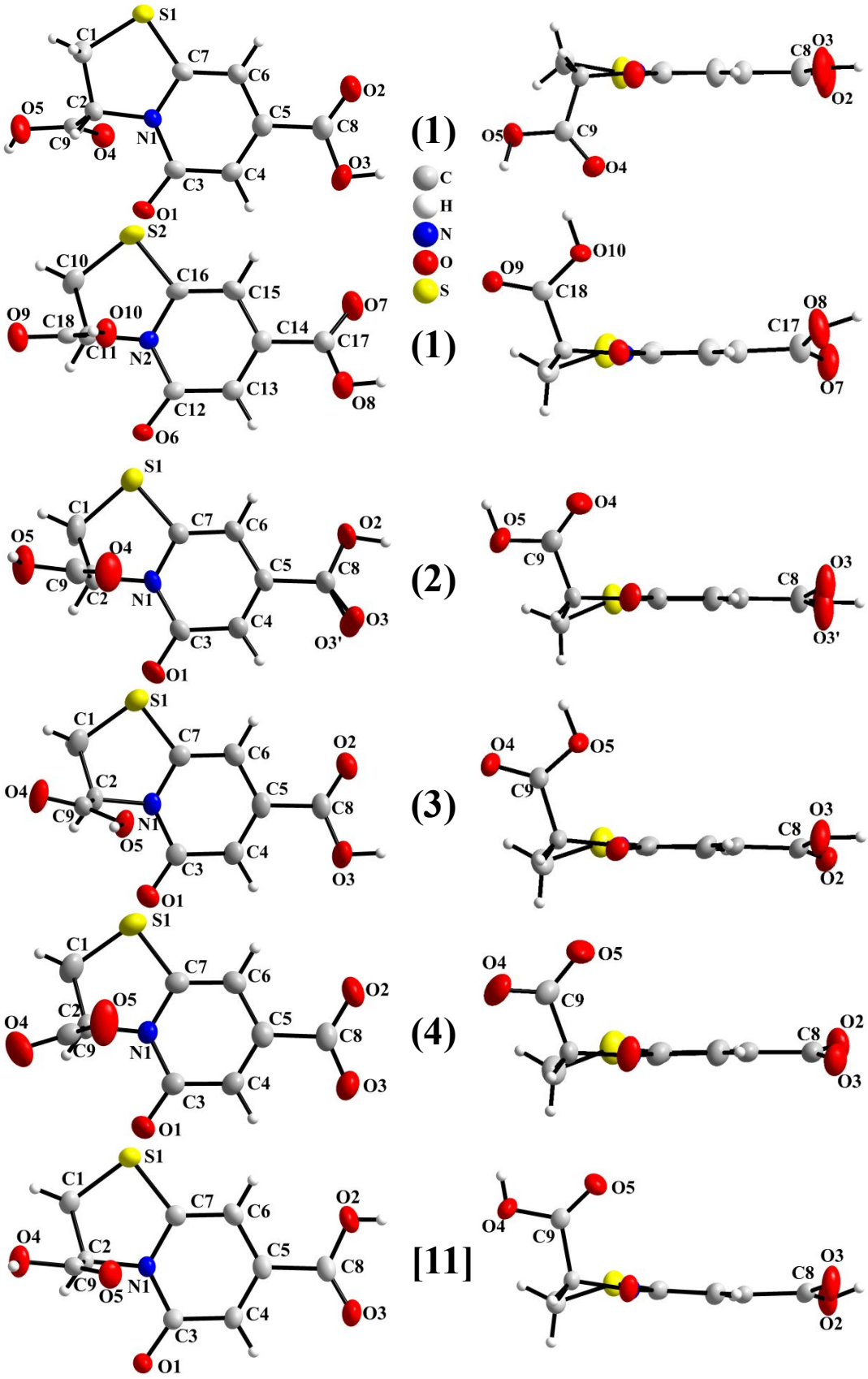

Figure S2. Comparison of TPDCA ligands in $C_9H_7NO_5S$, (**1**), (**2**), (**3**) and (**4**).

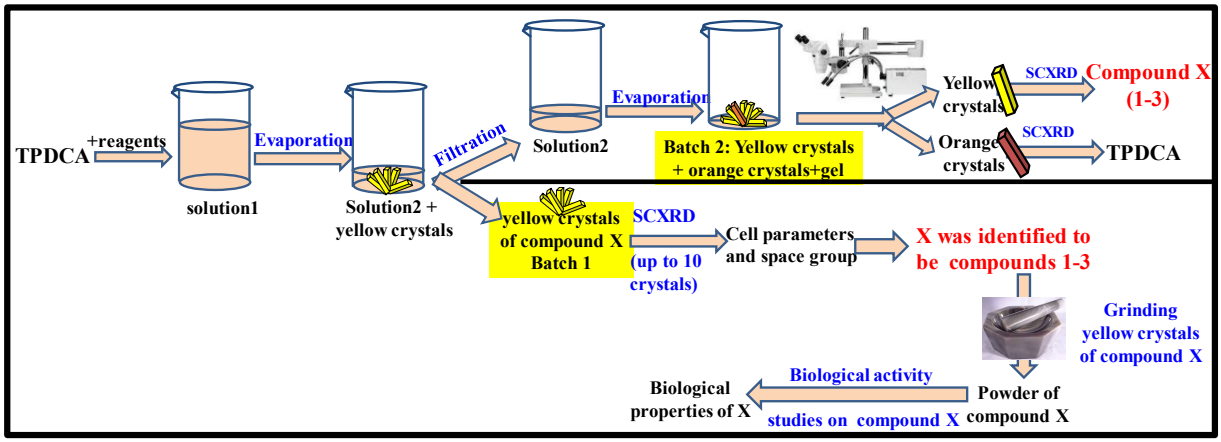

Figure S3. Synthesis and characterization processes for compounds 1-3.

Table S1 Atomic positions and isotopic displacement parameters (Å^2) for $C_{18}H_{14}N_2O_{10}S_2 \cdot H_2O$ (1).

Atom	Wyck.	*x*	*y*	*z*	*Ueq/iso (Å²)*
S1	2*a*	0.31668(9)	0.77426(7)	0.15543(3)	0.0427(2)
C1	2*a*	0.3585(3)	0.7866(3)	0.05190(12)	0.0343(7)
C2	2*a*	0.5855(3)	0.7338(2)	0.03922(12)	0.0258(6)
N1	2*a*	0.6464(3)	0.64548(17)	0.10593(9)	0.0239(5)
C3	2*a*	0.8246(3)	0.5627(2)	0.10415(12)	0.0277(6)
O1	2*a*	0.9266(2)	0.55904(16)	0.04241(9)	0.0363(5)
C4	2*a*	0.8784(4)	0.4895(2)	0.17326(12)	0.0332(7)
C5	2*a*	0.7596(4)	0.5041(2)	0.23811(13)	0.0335(7)
C6	2*a*	0.5813(4)	0.5914(2)	0.23756(13)	0.0383(8)
C7	2*a*	0.5282(3)	0.6609(2)	0.17047(12)	0.0297(7)
C8	2*a*	0.8164(4)	0.4268(3)	0.31176(14)	0.0427(8)
O2	2*a*	0.7268(4)	0.4414(3)	0.37082(11)	0.0753(9)
O3	2*a*	0.9750(4)	0.3403(2)	0.30391(11)	0.0663(8)
C9	2*a*	0.7504(3)	0.8468(2)	0.03401(12)	0.0265(6)
O4	2*a*	0.8887(2)	0.86972(16)	0.08381(9)	0.0356(5)
O5	2*a*	0.7228(3)	0.91615(18)	-0.03165(9)	0.0411(5)
S2	2*a*	0.11405(10)	0.80644(7)	0.34336(4)	0.0445(2)
C10	2*a*	0.1586(3)	0.8456(2)	0.44626(13)	0.0332(7)
C11	2*a*	-0.0594(3)	0.8885(2)	0.47422(12)	0.0227(6)
N2	2*a*	-0.1714(2)	0.95381(17)	0.40722(9)	0.0214(5)
C12	2*a*	-0.3450(3)	1.0374(2)	0.41813(12)	0.0229(6)
O6	2*a*	-0.3944(2)	1.05844(15)	0.48755(8)	0.0288(5)
C13	2*a*	-0.4524(3)	1.0867(2)	0.34962(12)	0.0287(6)
C14	2*a*	-0.3852(3)	1.0518(2)	0.27725(12)	0.0295(7)
C15	2*a*	-0.2057(3)	0.9665(3)	0.26895(13)	0.0341(7)
C16	2*a*	-0.1032(3)	0.9184(2)	0.33527(12)	0.0269(6)
C17	2*a*	-0.5076(4)	1.1022(3)	0.20539(13)	0.0364(8)
O7	2*a*	-0.4307(3)	1.1069(2)	0.14217(10)	0.0538(7)
O8	2*a*	-0.7035(3)	1.1371(2)	0.21981(10)	0.0563(7)
C18	2*a*	-0.1857(3)	0.7684(2)	0.50431(11)	0.0223(6)
O9	2*a*	-0.1242(2)	0.71032(17)	0.56430(9)	0.0359(5)
O10	2*a*	-0.3517(2)	0.73331(16)	0.46123(9)	0.0331(5)
O11	2*a*	0.0120(3)	0.17518(18)	0.10624(9)	0.0423(6)
H1c1	2*a*	0.2554	0.7305	0.0235	0.041207
H2c1	2*a*	0.3479	0.8802	0.0359	0.041207
H1c2	2*a*	0.5836	0.6863	-0.0098	0.030999
H1c4	2*a*	0.9994	0.4288	0.175	0.039879
H1c6	2*a*	0.4991	0.6019	0.2831	0.045981
H1c10	2*a*	0.2066	0.7652	0.4738	0.039816
H2c10	2*a*	0.2576	0.9203	0.4523	0.039816
H1c11	2*a*	-0.0433	0.9497	0.5178	0.027291
H1c13	2*a*	-0.5744	1.1456	0.3536	0.034413
H1c15	2*a*	-0.1576	0.9432	0.2183	0.040878
H1o3	2*a*	0.993(5)	0.295(3)	0.3533(9)	0.079613
H1o5	2*a*	0.849(2)	0.969(2)	-0.0406(15)	0.049333
H1o8	2*a*	-0.799(4)	1.145(3)	0.1741(10)	0.067551
H1o10	2*a*	-0.429(3)	0.6554(14)	0.4788(13)	0.039718
H1o11	2*a*	0.051(3)	0.116(2)	0.0644(10)	0.050784
H2o11	2*a*	-0.123(2)	0.140(2)	0.1218(13)	0.050784

Table S2 Anisotropic displacement parameters (Å^2) for $C_{18}H_{14}N_2O_{10}S_2 \cdot H_2O$ (1). The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S1	0.0343(3)	0.0599(4)	0.0348(3)	0.0211(3)	0.0099(2)	0.0105(3)
C1	0.0247(10)	0.0480(14)	0.0304(11)	0.0017(10)	0.0015(9)	0.0093(11)
C2	0.0257(10)	0.0310(12)	0.0209(10)	0.0008(9)	0.0010(8)	0.0013(9)
N1	0.0249(9)	0.0257(9)	0.0213(8)	0.0004(7)	0.0033(7)	0.0017(7)
C3	0.0303(11)	0.0265(11)	0.0268(11)	0.0025(9)	0.0054(9)	-0.0041(9)
O1	0.0383(9)	0.0429(10)	0.0289(8)	0.0123(7)	0.0122(7)	0.0013(7)
C4	0.0356(12)	0.0310(12)	0.0334(12)	0.0113(10)	0.0046(10)	0.0021(10)
C5	0.0376(12)	0.0345(13)	0.0283(12)	0.0055(10)	0.0004(9)	0.0016(10)
C6	0.0413(13)	0.0465(15)	0.0279(12)	0.0142(11)	0.0099(10)	0.0071(11)
C7	0.0283(11)	0.0344(13)	0.0267(11)	0.0032(9)	0.0067(9)	-0.0005(10)
C8	0.0515(15)	0.0452(15)	0.0312(13)	0.0116(13)	0.0021(11)	0.0052(11)
O2	0.0960(16)	0.0950(17)	0.0363(11)	0.0507(14)	0.0181(11)	0.0231(11)
O3	0.0821(14)	0.0771(15)	0.0403(11)	0.0469(12)	0.0076(10)	0.0208(10)
C9	0.0247(10)	0.0303(12)	0.0249(10)	0.0030(9)	0.0049(9)	-0.0008(9)
O4	0.0314(8)	0.0408(9)	0.0343(8)	-0.0042(7)	-0.0016(7)	0.0002(7)
O5	0.0407(9)	0.0472(10)	0.0353(9)	-0.0100(8)	0.0000(7)	0.0156(8)
S2	0.0388(3)	0.0565(4)	0.0392(3)	0.0244(3)	0.0131(3)	0.0030(3)
C10	0.0194(10)	0.0419(14)	0.0384(12)	0.0037(9)	0.0038(9)	0.0092(10)
C11	0.0187(10)	0.0225(11)	0.0268(11)	0.0001(8)	-0.0009(8)	0.0009(8)
N2	0.0180(8)	0.0219(9)	0.0243(8)	-0.0004(7)	0.0027(7)	0.0000(7)
C12	0.0213(9)	0.0195(10)	0.028(1)	-0.0010(8)	0.0039(8)	-0.0017(8)
O6	0.0294(7)	0.0335(9)	0.0239(7)	0.0095(6)	0.0037(6)	-0.0036(6)
C13	0.0257(10)	0.0307(12)	0.0298(11)	0.0033(9)	0.0023(9)	0.0000(9)
C14	0.0256(10)	0.0340(12)	0.0288(11)	0.0030(9)	0.0007(9)	0.003(1)
C15	0.0359(12)	0.0427(14)	0.0242(11)	0.0069(10)	0.0082(9)	-0.0016(10)
C16	0.0231(10)	0.0289(12)	0.0294(11)	0.0049(9)	0.0083(9)	-0.0007(9)
C17	0.0378(13)	0.0441(14)	0.0274(12)	0.0100(11)	0.0009(10)	-0.0002(10)
O7	0.0493(11)	0.0826(14)	0.0298(9)	0.0155(10)	0.0044(8)	0.0152(9)
O8	0.0412(10)	0.0936(16)	0.0336(9)	0.0268(11)	-0.0041(7)	0.004(1)
C18	0.0200(9)	0.0228(10)	0.0245(10)	0.0029(8)	0.0040(8)	-0.0043(9)
O9	0.0393(9)	0.0378(9)	0.0298(8)	-0.0104(7)	-0.0061(7)	0.0087(7)
O10	0.0280(8)	0.0336(9)	0.0370(8)	-0.0123(7)	-0.0049(6)	0.0089(7)
O11	0.0398(9)	0.0534(11)	0.0336(9)	-0.0014(8)	-0.0009(7)	-0.0029(8)

Table S3 Atomic coordinates and isotropic displacement parameters (in Å ^{2}) for $C_9H_7NO_5S \cdot C_5H_9NO$ (2).

Atom	Wyck.	Occ.	*x*	*y*	*z*	*Ueq/iso (Å^2)*
S1	4*e*	1	0.77725(4)	0.14992(7)	0.04353(3)	0.04368(19)
C1	4*e*	1	0.83628(13)	0.1443(3)	0.15942(11)	0.0389(6)
C2	4*e*	1	0.84778(12)	0.3569(2)	0.18695(10)	0.0304(5)
N1	4*e*	1	0.86730(9)	0.46034(19)	0.11386(7)	0.0268(4)
C3	4*e*	1	0.91386(11)	0.6380(2)	0.12524(9)	0.0276(5)
O1	4*e*	1	0.94195(9)	0.71154(19)	0.19892(7)	0.0398(4)
C4	4*e*	1	0.92656(11)	0.7220(2)	0.04825(10)	0.0299(5)
C5	4*e*	1	0.89299(11)	0.6324(2)	-0.03014(9)	0.0277(5)
C6	4*e*	1	0.84539(11)	0.4515(2)	-0.03864(9)	0.0312(5)
C7	4*e*	1	0.83348(11)	0.3700(2)	0.0348(1)	0.0287(5)
C8	4*e*	1	0.91078(13)	0.7325(3)	-0.10733(10)	0.0356(6)
O2	4*e*	1	0.88135(13)	0.6348(2)	-0.17862(8)	0.0593(6)
O3	4*e*	0.5	0.9297(5)	0.9091(14)	-0.1077(6)	0.061(2)
O3'	4*e*	0.5	0.9668(5)	0.8634(14)	-0.0997(6)	0.061(2)
C9	4*e*	1	0.76143(12)	0.4428(3)	0.20728(10)	0.0364(6)
O4	4*e*	1	0.71838(11)	0.5817(2)	0.17097(10)	0.0600(6)
O5	4*e*	1	0.74174(11)	0.3441(2)	0.26943(9)	0.0570(6)
N2	4*e*	1	0.49455(13)	1.1110(3)	0.12383(13)	0.0637(8)
C10	4*e*	1	0.41898(14)	1.0758(4)	0.14935(14)	0.0529(8)
O6	4*e*	1	0.40777(12)	0.9234(3)	0.18743(12)	0.0741(7)
C11	4*e*	1	0.35224(18)	1.2414(4)	0.12599(17)	0.0729(10)
C12	4*e*	1	0.3997(3)	1.3861(5)	0.0814(2)	0.1176(19)
C13	4*e*	1	0.4951(2)	1.3032(5)	0.0859(2)	0.0892(12)
C14	4*e*	1	0.57468(18)	0.9788(5)	0.14022(19)	0.0927(14)
H1c1	4*e*	1	0.79675	0.07922	0.18895	0.046689
H2c1	4*e*	1	0.89731	0.08511	0.16927	0.046689
H1c2	4*e*	1	0.89743	0.37007	0.24011	0.036523
H1c4	4*e*	1	0.95947	0.84427	0.05168	0.03592
H1c6	4*e*	1	0.82232	0.38824	-0.09396	0.037474
H1c11	4*e*	1	0.34409	1.29926	0.17782	0.087513
H2c11	4*e*	1	0.29447	1.19734	0.08605	0.087513
H1c12	4*e*	1	0.36349	1.39919	0.02176	0.141146
H2c12	4*e*	1	0.40714	1.50887	0.11167	0.141146
H1c13	4*e*	1	0.50121	1.28980	0.02829	0.107066
H2c13	4*e*	1	0.54306	1.38224	0.12382	0.107066
H1c14	4*e*	1	0.62306	1.02279	0.19020	0.111203
H2c14	4*e*	1	0.55506	0.84928	0.15056	0.111203
H3c14	4*e*	1	0.59885	0.97703	0.09074	0.111203
H1o2	4*e*	1	0.8967(16)	0.710(3)	-0.2230(11)	0.071184
H1o5	4*e*	1	0.6840(9)	0.388(3)	0.2791(15)	0.068453

Table S4 Anisotropic displacement parameters (in Å ^{2}) for $C_9H_7NO_5S \cdot C_5H_9NO$ (2). The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S1	0.0599(3)	0.0339(3)	0.0381(3)	-0.0125(2)	0.0151(2)	0.00074(19)
C1	0.0478(11)	0.0367(10)	0.0366(9)	0.0065(8)	0.0190(8)	0.0120(7)
C2	0.0339(9)	0.0360(9)	0.0229(7)	0.0051(7)	0.0106(6)	0.0088(6)
N1	0.0322(7)	0.0310(7)	0.0184(6)	0.0031(6)	0.0091(5)	0.0027(5)
C3	0.0316(8)	0.0308(8)	0.0214(7)	0.0022(6)	0.0092(6)	-0.0028(6)
O1	0.0525(7)	0.0469(7)	0.0216(5)	-0.0064(6)	0.0132(5)	-0.0103(5)
C4	0.0381(9)	0.0289(8)	0.0255(7)	-0.0028(7)	0.0133(6)	-0.0028(6)
C5	0.0326(8)	0.0312(8)	0.0209(7)	0.0015(6)	0.0100(6)	0.0004(6)
C6	0.0395(9)	0.0339(9)	0.0201(7)	-0.0031(7)	0.0083(6)	-0.0023(7)
C7	0.0338(8)	0.0273(8)	0.0249(7)	0.0007(6)	0.0082(6)	-0.0009(6)
C8	0.0488(10)	0.0363(10)	0.0241(8)	-0.0079(8)	0.0143(7)	-0.0023(7)
O2	0.1072(13)	0.0527(9)	0.0219(6)	-0.0304(8)	0.0245(7)	-0.0052(6)
O3	0.099(5)	0.055(4)	0.0325(16)	-0.036(3)	0.025(3)	-0.004(2)
O3'	0.099(5)	0.055(4)	0.0325(16)	-0.036(3)	0.025(3)	-0.004(2)
C9	0.0380(9)	0.0427(10)	0.0314(8)	0.0036(8)	0.0143(7)	0.0017(8)
O4	0.0588(9)	0.0616(9)	0.0686(10)	0.0288(8)	0.0326(8)	0.0233(8)
O5	0.0628(9)	0.0682(10)	0.0560(8)	0.0191(7)	0.0426(7)	0.0209(7)
N2	0.0454(10)	0.0810(14)	0.0680(12)	-0.0034(9)	0.0215(9)	0.0200(11)
C10	0.0457(11)	0.0655(14)	0.0504(11)	-0.0029(10)	0.0183(9)	-0.0005(11)
O6	0.0662(11)	0.0803(12)	0.0949(13)	0.0051(9)	0.054(1)	0.0197(10)
C11	0.0609(15)	0.0771(18)	0.0775(16)	0.0066(13)	0.0141(12)	-0.0080(14)
C12	0.095(2)	0.103(3)	0.155(4)	0.021(2)	0.035(2)	0.055(3)
C13	0.0761(18)	0.094(2)	0.093(2)	-0.0225(16)	0.0165(16)	0.0318(18)
C14	0.0567(16)	0.113(2)	0.122(3)	0.0101(16)	0.0476(16)	0.027(2)

Table S5 Atomic coordinates and isotropic displacement parameters (in Å ^{2}) for $C_9H_9NNaO_7PS$ (3).

Atom	Wyck.	*x*	*y*	*z*	*Ueq/iso (Å^2)*
S1	2*i*	-0.09202(6)	0.20599(5)	0.22679(4)	0.02380(13)
C1	2*i*	-0.0289(3)	0.38563(19)	0.16746(15)	0.0234(5)
C2	2*i*	0.2237(2)	0.43121(16)	0.17236(12)	0.0155(4)
N1	2*i*	0.3055(2)	0.38227(13)	0.27739(10)	0.0143(3)
C3	2*i*	0.5198(2)	0.44742(16)	0.32909(12)	0.0151(4)
O1	2*i*	0.63674(17)	0.55970(12)	0.29359(9)	0.0196(3)
C4	2*i*	0.5861(2)	0.37511(17)	0.42171(12)	0.0168(4)
C5	2*i*	0.4425(2)	0.25635(16)	0.45863(12)	0.0166(4)
C6	2*i*	0.2222(2)	0.19870(17)	0.40639(12)	0.0178(4)
C7	2*i*	0.1614(2)	0.26259(17)	0.31429(12)	0.0160(4)
C8	2*i*	0.5173(3)	0.18989(17)	0.56073(12)	0.0178(4)
O2	2*i*	0.38883(19)	0.10447(12)	0.61113(9)	0.0216(3)
O3	2*i*	0.7326(2)	0.23600(15)	0.58892(11)	0.0292(4)
H1o3	2*i*	0.775(3)	0.186(2)	0.6511(12)	0.035032
C9	2*i*	0.3029(2)	0.35693(16)	0.06394(12)	0.0145(4)
O4	2*i*	0.22575(19)	0.36912(14)	-0.03083(9)	0.0251(4)
O5	2*i*	0.45531(18)	0.28272(13)	0.08320(9)	0.0194(3)
H1o5	2*i*	0.496(3)	0.2381(19)	0.0116(8)	0.023239
Na1	2*i*	0.74862(9)	0.77456(7)	0.21683(5)	0.01767(19)
P1	2*i*	1.28913(6)	0.91595(4)	0.15022(3)	0.01623(12)
O6	2*i*	1.44820(19)	0.82207(14)	0.11022(10)	0.0248(4)
O7	2*i*	1.12522(17)	0.84898(13)	0.22887(9)	0.0206(3)
H1p1	2*i*	1.185(3)	0.934(2)	0.0595(16)	0.022(5)
H2p1	2*i*	1.411(3)	1.047(2)	0.1996(17)	0.029(5)
H1c1	2*i*	-0.0923	0.3675	0.0885	0.028038
H2c1	2*i*	-0.0779	0.4628	0.2158	0.028038
H1c2	2*i*	0.28	0.5401	0.1747	0.01859
H1c4	2*i*	0.7351	0.4108	0.4589	0.02016
H1c6	2*i*	0.1196	0.118	0.4344	0.021339

Table S6 Anisotropic displacement parameters (in Å ^{2}) for $C_9H_9NNaO_7PS$ (3). The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S1	0.01633	0.03154	0.02265	0.00330	-0.00051	0.00719
C1	0.01864	0.03412	0.02334	0.01435	0.00531	0.01004
C2	0.01852	0.01911	0.01187	0.00912	0.00279	0.00449
N1	0.01716	0.01739	0.01042	0.00762	0.00348	0.00249
C3	0.01763	0.01781	0.01072	0.00662	0.00411	0.00008
O1	0.02218	0.02004	0.01664	0.00353	0.00511	0.00481
C4	0.01852	0.02148	0.01061	0.00587	0.00129	0.00173
C5	0.02267	0.01985	0.00971	0.00992	0.00344	0.00198
C6	0.02126	0.01814	0.01433	0.00428	0.00408	0.00384
C7	0.01545	0.01884	0.01409	0.00533	0.00351	0.00145
C8	0.02457	0.01934	0.01123	0.00863	0.00262	0.00268
O2	0.02893	0.02220	0.01520	0.00738	0.00391	0.00566
O3	0.02388	0.04326	0.02346	0.00783	0.00009	0.01805
C9	0.01406	0.01681	0.01365	0.00414	0.00281	0.00452
O4	0.03178	0.03747	0.01229	0.02072	0.00059	0.00467
O5	0.02134	0.02817	0.01356	0.01498	0.00372	0.00390
Na1	0.01393	0.02398	0.01579	0.00471	0.00257	0.00505
P1	0.01594	0.02108	0.01488	0.00884	0.00445	0.00502
O6	0.02615	0.03961	0.01452	0.02169	0.00313	0.00023
O7	0.01336	0.03096	0.01804	0.00414	0.00191	0.00854

Table S7 Atomic coordinates and isotropic displacement parameters (in Å ^{2}) for $(C_9H_5NO_5S)(NH_4)_2(H_2O)$ (4).

Atom	Wyck.	*x*	*y*	*z*	*Ueq/iso (Å^2)*
S1	2*i*	0.49810(9)	0.18604(5)	1.04691(4)	0.03142(18)
N1	2*i*	0.3687(2)	0.34983(13)	0.82931(12)	0.0185(5)
O1	2*i*	0.2313(2)	0.45441(12)	0.63444(12)	0.0301(5)
C1	2*i*	0.2147(3)	0.15737(18)	1.00826(17)	0.0297(7)
O5	2*i*	0.5478(3)	0.14917(15)	0.74543(15)	0.0456(6)
C5	2*i*	0.6795(3)	0.54760(16)	0.77539(16)	0.0206(6)
O2	2*i*	0.9981(2)	0.64499(13)	0.81862(13)	0.0335(5)
N2	2*i*	0.9159(3)	0.30990(15)	0.56994(15)	0.0303(6)
C2	2*i*	0.2221(3)	0.23365(15)	0.86175(15)	0.0194(6)
O4	2*i*	0.1833(2)	0.07612(13)	0.76854(14)	0.0391(6)
O3	2*i*	0.8151(2)	0.76459(12)	0.64639(12)	0.0317(5)
N3	2*i*	0.7037(3)	0.13049(15)	0.32850(15)	0.0275(6)
C3	2*i*	0.3694(3)	0.45441(16)	0.71194(15)	0.0205(6)
C4	2*i*	0.5323(3)	0.55578(16)	0.68749(16)	0.0225(6)
C9	2*i*	0.3270(3)	0.14634(16)	0.78282(15)	0.0222(6)
C8	2*i*	0.8464(3)	0.66080(17)	0.74578(17)	0.0227(6)
C6	2*i*	0.6770(3)	0.43624(16)	0.89294(16)	0.0220(6)
O6	2*i*	0.7939(3)	0.03548(13)	0.58466(12)	0.0352(5)
C7	2*i*	0.5220(3)	0.33834(16)	0.91607(15)	0.0197(6)
H1c1	2*i*	0.2033	0.0632	1.0279	0.035614
H2c1	2*i*	0.0851	0.1942	1.0536	0.035614
H1c2	2*i*	0.0627	0.2606	0.84	0.023262
H1c4	2*i*	0.5392	0.6319	0.6073	0.027023
H1c6	2*i*	0.781	0.4294	0.9548	0.026402
H1n3	2*i*	0.7166(15)	0.0660(7)	0.2988(10)	0.032949
H2n3	2*i*	0.7411	0.0991	0.407	0.032949
H3n3	2*i*	0.8005	0.1931	0.2788	0.032949
H4n3	2*i*	0.5568	0.1638	0.3295	0.032949
H1n2	2*i*	0.9881(13)	0.2557(8)	0.5330(9)	0.036419
H2n2	2*i*	0.8488	0.3778	0.513	0.036419
H3n2	2*i*	0.8067	0.2675	0.6325	0.036419
H4n2	2*i*	1.0201	0.3386	0.6013	0.036419
H1o6	2*i*	0.816(3)	-0.0598(5)	0.6158(15)	0.042264
H2o6	2*i*	0.688(3)	0.0532(16)	0.6524(12)	0.042264

Table S8 Anisotropic displacement parameters (in Å ^{2}) for $(C_9H_5NO_5S)(NH_4)_2(H_2O)$ (4). The anisotropic displacement factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11}+...+2hka^*b^*U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S1	0.0412(3)	0.0260(3)	0.0219(2)	-0.0056(2)	-0.00834(19)	-0.00041(17)
N1	0.0208(7)	0.0148(6)	0.0209(7)	-0.0021(5)	-0.0030(6)	-0.0072(5)
O1	0.0375(7)	0.0257(6)	0.0291(7)	-0.0080(5)	-0.0163(6)	-0.0058(5)
C1	0.0362(10)	0.0285(9)	0.0225(9)	-0.0117(8)	0.0043(8)	-0.0081(7)
O5	0.0367(9)	0.0465(9)	0.0614(10)	-0.0123(7)	0.0203(7)	-0.0370(8)
C5	0.0192(8)	0.0189(8)	0.0258(8)	-0.0003(7)	-0.0007(7)	-0.0115(7)
O2	0.0288(7)	0.0339(7)	0.0417(8)	-0.0100(6)	-0.0095(6)	-0.0139(6)
N2	0.0355(9)	0.0271(8)	0.0310(8)	-0.0053(7)	-0.0077(7)	-0.0113(7)
C2	0.0188(8)	0.0161(7)	0.0235(8)	-0.0039(6)	-0.0006(6)	-0.0077(6)
O4	0.0403(8)	0.0352(8)	0.0561(9)	-0.0027(6)	-0.0141(7)	-0.0296(7)
O3	0.0356(8)	0.0221(6)	0.0350(7)	-0.0086(6)	-0.0041(6)	-0.0063(5)
N3	0.0272(9)	0.0270(8)	0.0318(8)	-0.0042(6)	-0.0069(7)	-0.0129(6)
C3	0.0244(9)	0.0166(8)	0.0211(8)	0.0003(7)	-0.0046(7)	-0.0076(6)
C4	0.0283(9)	0.0164(8)	0.0217(8)	-0.0032(7)	-0.0044(7)	-0.0048(6)
C9	0.0291(9)	0.0172(8)	0.0189(8)	-0.0006(7)	-0.0037(7)	-0.0053(6)
C8	0.0208(8)	0.0206(8)	0.0293(9)	-0.0026(7)	0.0014(7)	-0.0135(7)
C6	0.0232(9)	0.0216(8)	0.0233(8)	-0.0001(7)	-0.0068(7)	-0.0094(7)
O6	0.0479(9)	0.0272(7)	0.0302(7)	-0.0028(6)	0.0036(6)	-0.0135(6)
C7	0.0220(8)	0.0194(8)	0.0179(7)	0.0013(7)	-0.0030(7)	-0.0074(6)